Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:00 PM GMT

PDB ID	:	1DLO
Title	:	HUMAN IMMUNODEFICIENCY VIRUS TYPE 1
Authors	:	Hsiou, Y.; Ding, J.; Das, K.; Hughes, S.; Arnold, E.
Deposited on	:	1996-04-17
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

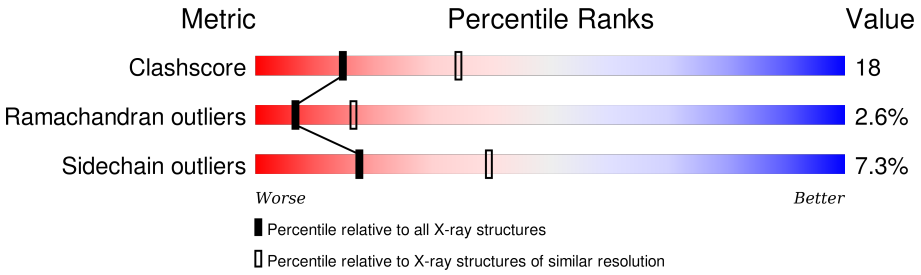
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	556	59% 37%
2	B	427	54% 39%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7691 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	0	0
			4370	2835	727	802	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 2 is a protein called HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	415	Total	C	N	O	S	0	0	0
			3321	2163	549	604	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED	UNP P03366

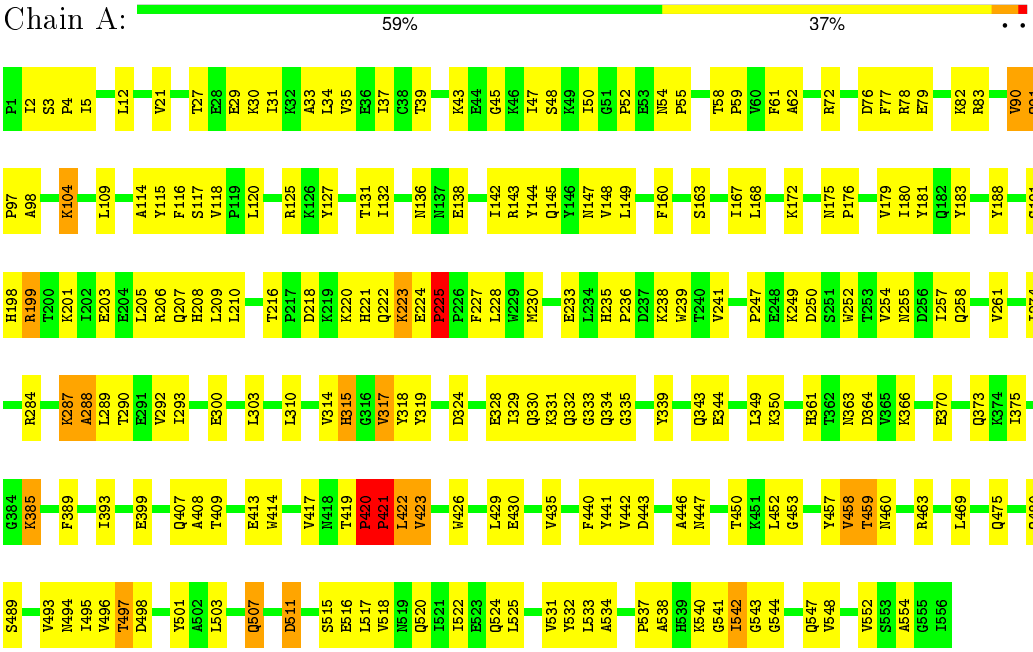
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

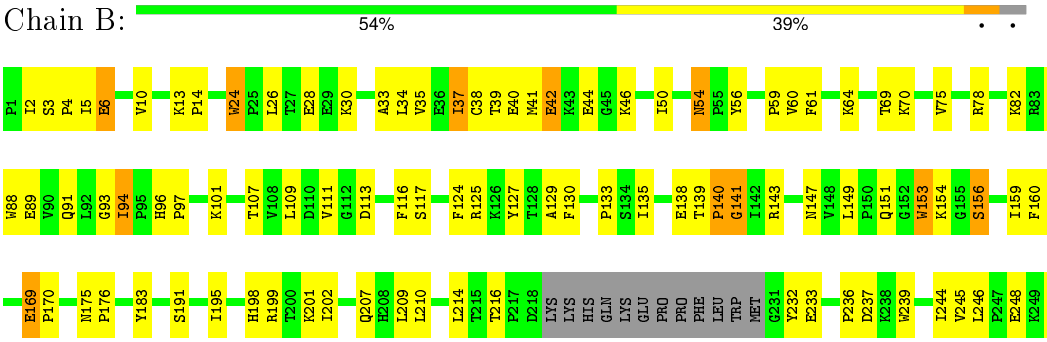
• Molecule 1: HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 REVERSE TRANSCRIPTASE

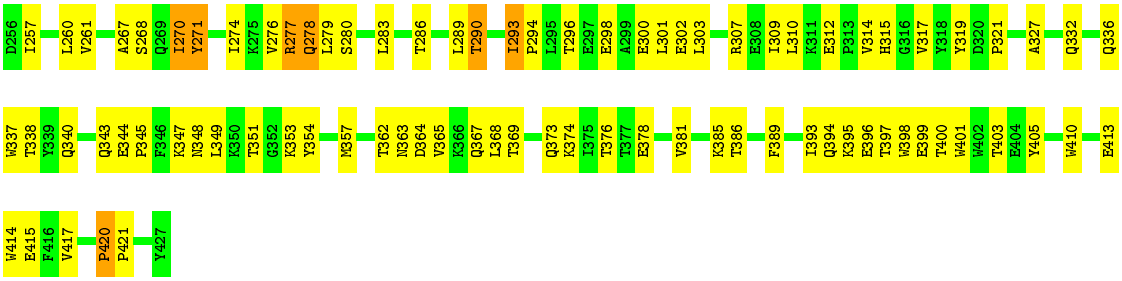
Chain A:



• Molecule 2: HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 REVERSE TRANSCRIPTASE

Chain B:




D256 I257 L260 V261 A267 S268 Q269 I270 Y271 I274 K275 V276 R277 Q278 L279 S280 L283 T286 L289 T290 I293 P294 L295 T296 E297 E298 A299 E300 L301 E302 L303 R307 E308 I309 L310 K311 E312 P313 V314 H315 G316 V317 Y318 Y319 D320 P321 A327 Q332 Q336
W337 T338 Y339 Q340 Q343 E344 P345 F346 K347 N348 L349 K350 T351 G352 K353 Y354 M357 T362 N363 D364 V365 K366 Q367 L368 T369 Q373 K374 I375 T376 T377 E378 V381 K385 T386 F389 I393 Q394 K395 E396 T397 W398 E399 T400 W401 W402 T403 E404 Y405 W410 E413
W414 E415 F416 V417 P420 P421 Y427

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	235.50Å 70.30Å 93.30Å 90.00° 106.10° 90.00°	Depositor
Resolution (Å)	8.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.249 , 0.336	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7691	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.69	0/4486	0.87	5/6119 (0.1%)
2	B	0.72	0/3415	0.90	1/4652 (0.0%)
All	All	0.70	0/7901	0.89	6/10771 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	2
All	All	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	90	VAL	N-CA-C	5.73	126.48	111.00
1	A	91	GLN	N-CA-C	5.54	125.95	111.00
1	A	136	ASN	N-CA-C	-5.26	96.80	111.00
2	B	54	ASN	N-CA-C	-5.25	96.82	111.00
1	A	120	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	421	PRO	CA-N-CD	-5.08	104.39	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	501	TYR	Sidechain
2	B	127	TYR	Sidechain
2	B	183	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4370	0	4315	151	0
2	B	3321	0	3293	135	0
All	All	7691	0	7608	270	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (270) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:LEU:HD21	2:B:303:LEU:HD21	1.58	0.86
1:A:420:PRO:HB3	1:A:421:PRO:HD2	1.57	0.85
1:A:420:PRO:CB	1:A:421:PRO:HD2	2.06	0.85
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.57	0.83
2:B:255:ASN:HB2	2:B:289:LEU:HB3	1.61	0.80
2:B:348:ASN:HD22	2:B:351:THR:HG22	1.45	0.80
1:A:435:VAL:HA	2:B:290:THR:HG21	1.64	0.80
2:B:198:HIS:O	2:B:202:ILE:HG12	1.84	0.78
1:A:228:LEU:HD23	1:A:233:GLU:HG3	1.66	0.77
1:A:543:GLY:HA2	2:B:283:LEU:O	1.84	0.77
2:B:250:ASP:OD2	2:B:303:LEU:HD13	1.84	0.76
1:A:442:VAL:HG13	1:A:481:ALA:HB1	1.69	0.75
1:A:50:ILE:HG21	1:A:145:GLN:HE21	1.51	0.74
2:B:209:LEU:HD22	2:B:214:LEU:HD12	1.68	0.74
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.71	0.72
1:A:199:ARG:HD3	1:A:199:ARG:O	1.91	0.71
1:A:34:LEU:HB3	1:A:132:ILE:HD12	1.72	0.71
1:A:276:VAL:HG12	1:A:280:SER:OG	1.92	0.69
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.74	0.68
2:B:195:ILE:HG12	2:B:199:ARG:NE	2.07	0.68
2:B:109:LEU:HD22	2:B:216:THR:HG21	1.75	0.68
1:A:206:ARG:HH22	1:A:218:ASP:HA	1.60	0.67
2:B:195:ILE:HG12	2:B:199:ARG:HE	1.59	0.67
1:A:532:TYR:CE1	1:A:534:ALA:HB2	2.31	0.66
1:A:116:PHE:O	1:A:148:VAL:HG21	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:TRP:CZ3	2:B:403:THR:HG21	2.32	0.65
1:A:457:TYR:O	1:A:458:VAL:HG23	1.98	0.64
1:A:109:LEU:HD22	1:A:216:THR:HG21	1.80	0.63
1:A:223:LYS:HD2	1:A:227:PHE:HZ	1.64	0.62
2:B:89:GLU:O	2:B:91:GLN:HG2	1.99	0.62
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.80	0.62
1:A:257:ILE:HD12	1:A:293:ILE:HD12	1.81	0.62
2:B:140:PRO:O	2:B:141:GLY:O	2.17	0.61
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.81	0.61
1:A:199:ARG:HE	1:A:220:LYS:HE2	1.64	0.61
2:B:348:ASN:ND2	2:B:351:THR:HG22	2.15	0.61
2:B:209:LEU:HB3	2:B:214:LEU:HB2	1.81	0.61
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.00	0.61
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.35	0.61
2:B:191:SER:OG	2:B:198:HIS:CD2	2.54	0.60
2:B:40:GLU:O	2:B:44:GLU:HG3	2.01	0.60
1:A:541:GLY:O	2:B:280:SER:HB3	2.02	0.60
2:B:298:GLU:O	2:B:301:LEU:HB3	2.02	0.60
2:B:420:PRO:HB2	2:B:421:PRO:CD	2.32	0.60
1:A:426:TRP:HE1	1:A:511:ASP:HB2	1.67	0.59
1:A:518:VAL:O	1:A:522:ILE:HG12	2.02	0.59
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.83	0.59
2:B:28:GLU:HG3	2:B:135:ILE:CD1	2.33	0.59
1:A:168:LEU:HD13	1:A:180:ILE:HG21	1.85	0.58
2:B:395:LYS:O	2:B:399:GLU:HG3	2.03	0.58
2:B:363:ASN:O	2:B:367:GLN:HG3	2.03	0.58
1:A:331:LYS:HG2	1:A:332:GLN:N	2.17	0.58
2:B:24:TRP:HH2	2:B:61:PHE:CD1	2.22	0.58
2:B:207:GLN:OE1	2:B:210:LEU:HD23	2.04	0.58
1:A:235:HIS:HB2	1:A:238:LYS:O	2.03	0.58
1:A:203:GLU:O	1:A:207:GLN:HB2	2.03	0.57
2:B:254:VAL:HA	2:B:257:ILE:HD12	1.86	0.57
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.05	0.57
2:B:244:ILE:HB	2:B:310:LEU:HD22	1.86	0.57
2:B:420:PRO:HB2	2:B:421:PRO:HD2	1.86	0.57
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.86	0.57
1:A:441:TYR:O	1:A:548:VAL:HG21	2.04	0.57
1:A:495:ILE:HD12	1:A:495:ILE:H	1.70	0.57
1:A:495:ILE:HG22	1:A:496:VAL:N	2.20	0.57
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.87	0.57
1:A:252:TRP:O	1:A:292:VAL:HG13	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:THR:HA	2:B:232:TYR:O	2.04	0.57
1:A:419:THR:O	1:A:422:LEU:HD23	2.04	0.56
2:B:354:TYR:CD1	2:B:374:LYS:HD2	2.41	0.56
1:A:493:VAL:HG22	1:A:494:ASN:N	2.21	0.56
2:B:354:TYR:CE1	2:B:374:LYS:HD2	2.40	0.56
1:A:366:LYS:O	1:A:370:GLU:HG3	2.05	0.56
1:A:132:ILE:HB	1:A:142:ILE:HB	1.88	0.56
2:B:296:THR:O	2:B:300:GLU:HG2	2.05	0.56
1:A:225:PRO:HB3	1:A:236:PRO:HD3	1.88	0.56
2:B:41:MET:HG3	2:B:46:LYS:HD2	1.87	0.56
2:B:24:TRP:CH2	2:B:61:PHE:CD1	2.93	0.55
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.42	0.55
1:A:98:ALA:HB1	1:A:349:LEU:HB3	1.88	0.55
1:A:276:VAL:HG12	1:A:280:SER:HG	1.72	0.55
2:B:260:LEU:HD23	2:B:279:LEU:HD13	1.89	0.54
1:A:458:VAL:HG12	2:B:286:THR:HG21	1.88	0.54
2:B:396:GLU:O	2:B:400:THR:HG23	2.07	0.54
2:B:64:LYS:HE2	2:B:69:THR:H	1.73	0.54
1:A:131:THR:HG23	1:A:143:ARG:HG2	1.88	0.54
1:A:435:VAL:CA	2:B:290:THR:HG21	2.36	0.54
2:B:393:ILE:HG21	2:B:398:TRP:HB2	1.89	0.54
1:A:417:VAL:O	1:A:417:VAL:HG13	2.08	0.54
1:A:115:TYR:O	1:A:149:LEU:HB2	2.07	0.54
2:B:64:LYS:HE2	2:B:69:THR:N	2.23	0.54
1:A:261:VAL:HG13	1:A:276:VAL:CG1	2.37	0.54
1:A:125:ARG:HB3	1:A:145:GLN:OE1	2.08	0.54
1:A:495:ILE:N	1:A:495:ILE:HD12	2.24	0.53
1:A:319:TYR:HE1	1:A:343:GLN:NE2	2.07	0.53
1:A:344:GLU:HA	1:A:344:GLU:OE1	2.07	0.53
1:A:503:LEU:O	1:A:507:GLN:HB2	2.07	0.53
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.91	0.53
1:A:333:GLY:O	1:A:335:GLY:N	2.42	0.53
1:A:520:GLN:O	1:A:524:GLN:HG2	2.09	0.53
1:A:317:VAL:HG13	1:A:318:TYR:N	2.22	0.52
2:B:96:HIS:CE1	2:B:381:VAL:O	2.63	0.52
2:B:332:GLN:O	2:B:336:GLN:HB3	2.08	0.52
1:A:407:GLN:NE2	2:B:417:VAL:O	2.43	0.52
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.91	0.52
2:B:376:THR:HG23	2:B:386:THR:HG22	1.92	0.52
1:A:480:GLN:O	1:A:483:TYR:HB3	2.10	0.52
1:A:90:VAL:HG23	1:A:91:GLN:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:ILE:HG23	2:B:294:PRO:HD2	1.92	0.51
2:B:139:THR:O	2:B:141:GLY:N	2.44	0.51
2:B:26:LEU:HD12	2:B:133:PRO:CG	2.40	0.51
1:A:27:THR:O	1:A:31:ILE:HG13	2.11	0.51
2:B:338:THR:HA	2:B:353:LYS:HA	1.90	0.51
1:A:223:LYS:HD2	1:A:227:PHE:CZ	2.44	0.51
1:A:389:PHE:O	1:A:414:TRP:HA	2.11	0.51
2:B:101:LYS:O	2:B:236:PRO:HB2	2.11	0.51
2:B:160:PHE:CD2	2:B:160:PHE:O	2.63	0.51
1:A:440:PHE:CZ	1:A:489:SER:HB2	2.46	0.51
2:B:278:GLN:HB2	2:B:302:GLU:OE1	2.11	0.51
1:A:183:TYR:CD2	1:A:230:MET:SD	3.04	0.50
1:A:350:LYS:HE2	1:A:378:GLU:OE2	2.11	0.50
2:B:111:VAL:HG12	2:B:111:VAL:O	2.11	0.50
1:A:319:TYR:OH	1:A:385:LYS:HD3	2.12	0.50
2:B:3:SER:O	2:B:5:ILE:HG13	2.11	0.50
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.77	0.50
2:B:191:SER:OG	2:B:198:HIS:HD2	1.94	0.50
1:A:442:VAL:CG1	1:A:443:ASP:N	2.75	0.50
1:A:59:PRO:HB2	1:A:76:ASP:HB3	1.94	0.50
2:B:257:ILE:O	2:B:261:VAL:HG23	2.11	0.49
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.94	0.49
1:A:27:THR:OG1	1:A:30:LYS:HG3	2.12	0.49
2:B:271:TYR:HD1	2:B:271:TYR:H	1.59	0.49
2:B:175:ASN:OD1	2:B:201:LYS:NZ	2.44	0.49
1:A:459:THR:HG23	1:A:463:ARG:HB3	1.94	0.49
1:A:61:PHE:CE1	1:A:290:THR:HG23	2.48	0.49
2:B:314:VAL:HG12	2:B:315:HIS:N	2.28	0.49
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.43	0.49
1:A:35:VAL:O	1:A:39:THR:HG23	2.11	0.49
1:A:446:ALA:HA	1:A:453:GLY:HA3	1.95	0.49
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.95	0.48
2:B:296:THR:HB	2:B:298:GLU:HG2	1.95	0.48
1:A:191:SER:OG	1:A:198:HIS:HD2	1.97	0.48
1:A:3:SER:OG	1:A:5:ILE:HG22	2.13	0.48
2:B:2:ILE:HA	2:B:117:SER:O	2.13	0.48
2:B:357:MET:CB	2:B:367:GLN:NE2	2.76	0.48
1:A:379:SER:HA	1:A:383:TRP:CE3	2.49	0.48
1:A:435:VAL:HG13	2:B:290:THR:HG21	1.95	0.48
2:B:85:GLN:O	2:B:85:GLN:HG3	2.14	0.48
1:A:175:ASN:N	1:A:176:PRO:HD3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:TYR:CD1	2:B:271:TYR:N	2.82	0.48
1:A:2:ILE:HD11	1:A:45:GLY:O	2.14	0.47
2:B:54:ASN:HD21	2:B:129:ALA:HB2	1.78	0.47
1:A:94:ILE:O	1:A:94:ILE:HG13	2.14	0.47
1:A:239:TRP:HZ2	1:A:349:LEU:O	1.96	0.47
1:A:163:SER:O	1:A:167:ILE:HG13	2.14	0.47
1:A:319:TYR:CE1	1:A:343:GLN:NE2	2.82	0.47
1:A:109:LEU:HD22	1:A:216:THR:CG2	2.43	0.47
1:A:324:ASP:O	1:A:343:GLN:HG2	2.15	0.47
1:A:361:HIS:HD2	1:A:518:VAL:HG11	1.80	0.47
2:B:267:ALA:O	2:B:270:ILE:N	2.47	0.47
1:A:47:ILE:HD12	1:A:144:TYR:CD1	2.50	0.47
2:B:37:ILE:HG22	2:B:41:MET:HE3	1.96	0.47
2:B:343:GLN:HG3	2:B:349:LEU:HD11	1.95	0.47
2:B:30:LYS:O	2:B:34:LEU:HD12	2.15	0.47
2:B:54:ASN:ND2	2:B:129:ALA:HB2	2.29	0.47
2:B:89:GLU:O	2:B:91:GLN:N	2.48	0.47
2:B:35:VAL:O	2:B:39:THR:HG23	2.15	0.47
1:A:430:GLU:HG2	1:A:531:VAL:O	2.15	0.46
1:A:50:ILE:HG21	1:A:145:GLN:NE2	2.24	0.46
1:A:254:VAL:HB	1:A:289:LEU:HA	1.98	0.46
1:A:460:ASN:HA	2:B:286:THR:O	2.16	0.46
2:B:420:PRO:CB	2:B:421:PRO:CD	2.93	0.46
1:A:228:LEU:CD2	1:A:233:GLU:HG3	2.42	0.46
1:A:222:GLN:O	1:A:224:GLU:N	2.49	0.46
1:A:532:TYR:HE1	1:A:534:ALA:HB2	1.79	0.46
1:A:241:VAL:CG2	1:A:314:VAL:HB	2.46	0.46
2:B:195:ILE:HG23	2:B:199:ARG:HH21	1.81	0.46
1:A:426:TRP:NE1	1:A:511:ASP:HB2	2.31	0.46
1:A:247:PRO:HB2	1:A:249:LYS:HE3	1.98	0.46
2:B:124:PHE:CE2	2:B:153:TRP:CZ2	3.04	0.46
2:B:254:VAL:HB	2:B:289:LEU:HA	1.98	0.46
1:A:225:PRO:O	1:A:227:PHE:N	2.49	0.45
2:B:78:ARG:O	2:B:82:LYS:HG3	2.16	0.45
2:B:56:TYR:O	2:B:143:ARG:NH2	2.49	0.45
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.38	0.45
2:B:125:ARG:HD3	2:B:147:ASN:HA	1.99	0.45
2:B:293:ILE:HG23	2:B:294:PRO:CD	2.47	0.45
1:A:429:LEU:HD23	1:A:531:VAL:HB	1.98	0.45
1:A:181:TYR:CE2	2:B:138:GLU:HA	2.52	0.45
2:B:33:ALA:O	2:B:37:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ILE:O	1:A:208:HIS:NE2	2.49	0.45
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.52	0.45
2:B:5:ILE:HG22	2:B:6:GLU:O	2.17	0.45
2:B:13:LYS:HB3	2:B:14:PRO:HD2	1.99	0.45
1:A:515:SER:OG	1:A:518:VAL:HG23	2.17	0.45
1:A:221:HIS:HB3	1:A:227:PHE:CD1	2.52	0.45
1:A:458:VAL:O	1:A:458:VAL:HG12	2.15	0.44
2:B:283:LEU:HD23	2:B:283:LEU:HA	1.79	0.44
2:B:124:PHE:CZ	2:B:153:TRP:CZ2	3.04	0.44
2:B:169:GLU:HG2	2:B:170:PRO:N	2.32	0.44
1:A:172:LYS:HE2	1:A:180:ILE:HB	2.00	0.44
1:A:542:ILE:CG2	2:B:283:LEU:HD13	2.47	0.44
1:A:255:ASN:HD22	1:A:289:LEU:HD13	1.83	0.44
1:A:328:GLU:O	1:A:339:TYR:HA	2.18	0.44
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.99	0.44
2:B:38:CYS:O	2:B:42:GLU:HB2	2.17	0.44
1:A:495:ILE:CG2	1:A:496:VAL:N	2.81	0.44
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.82	0.44
1:A:315:HIS:ND1	1:A:315:HIS:N	2.66	0.43
2:B:327:ALA:HA	2:B:340:GLN:O	2.18	0.43
2:B:94:ILE:H	2:B:94:ILE:HD13	1.82	0.43
1:A:79:GLU:HG3	1:A:83:ARG:HE	1.83	0.43
1:A:361:HIS:CD2	1:A:518:VAL:HG11	2.53	0.43
2:B:41:MET:HG2	2:B:46:LYS:HB2	2.01	0.43
2:B:376:THR:CG2	2:B:386:THR:HG22	2.47	0.43
2:B:270:ILE:HG22	2:B:271:TYR:CD1	2.53	0.43
2:B:362:THR:HA	2:B:367:GLN:HE21	1.83	0.43
1:A:241:VAL:HG23	1:A:314:VAL:HB	1.99	0.43
2:B:317:VAL:HG12	2:B:347:LYS:HB3	2.00	0.43
1:A:78:ARG:HD3	1:A:258:GLN:NE2	2.33	0.43
1:A:181:TYR:HB2	1:A:188:TYR:HB3	2.00	0.43
2:B:111:VAL:CG1	2:B:111:VAL:O	2.67	0.43
2:B:160:PHE:HE2	2:B:164:MET:HE2	1.84	0.42
1:A:205:LEU:O	1:A:209:LEU:HG	2.19	0.42
2:B:96:HIS:HE1	2:B:381:VAL:O	2.01	0.42
1:A:79:GLU:HG3	1:A:83:ARG:HH21	1.84	0.42
1:A:544:GLY:O	1:A:547:GLN:N	2.51	0.42
1:A:480:GLN:CA	1:A:517:LEU:HD21	2.50	0.42
1:A:498:ASP:HB2	1:A:538:ALA:HB2	2.00	0.42
2:B:116:PHE:CZ	2:B:151:GLN:HG3	2.54	0.42
2:B:93:GLY:HA2	2:B:161:GLN:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:337:TRP:CZ3	2:B:368:LEU:HD13	2.54	0.42
1:A:78:ARG:O	1:A:82:LYS:HG3	2.18	0.42
1:A:540:LYS:HZ3	2:B:276:VAL:HG11	1.85	0.42
2:B:24:TRP:NE1	2:B:59:PRO:HB3	2.34	0.42
1:A:33:ALA:O	1:A:37:ILE:HG13	2.19	0.42
1:A:515:SER:HB3	1:A:518:VAL:CG2	2.49	0.42
2:B:26:LEU:HD12	2:B:133:PRO:CD	2.49	0.42
2:B:389:PHE:O	2:B:415:GLU:N	2.52	0.42
2:B:309:ILE:HD12	2:B:312:GLU:OE2	2.20	0.42
2:B:246:LEU:HD21	2:B:310:LEU:HD11	2.02	0.42
1:A:175:ASN:HD21	1:A:201:LYS:NZ	2.18	0.42
2:B:50:ILE:CD1	2:B:54:ASN:HD22	2.33	0.42
1:A:2:ILE:HA	1:A:117:SER:O	2.20	0.42
2:B:107:THR:OG1	2:B:198:HIS:HE1	2.03	0.41
1:A:118:VAL:O	1:A:148:VAL:HG22	2.20	0.41
1:A:58:THR:HG21	1:A:77:PHE:CD1	2.55	0.41
1:A:220:LYS:HE3	1:A:222:GLN:HG3	2.03	0.41
2:B:195:ILE:HG13	2:B:233:GLU:OE1	2.21	0.41
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.90	0.41
2:B:344:GLU:HA	2:B:345:PRO:HD2	1.87	0.41
1:A:537:PRO:HG2	1:A:542:ILE:HD11	2.01	0.41
1:A:482:ILE:HD11	1:A:497:THR:HG21	2.02	0.41
2:B:277:ARG:HG2	2:B:278:GLN:NE2	2.35	0.41
2:B:410:TRP:O	2:B:410:TRP:CE3	2.74	0.41
1:A:373:GLN:NE2	2:B:397:THR:HG23	2.35	0.41
1:A:21:VAL:HB	1:A:59:PRO:HD3	2.02	0.41
1:A:142:ILE:N	1:A:142:ILE:HD13	2.36	0.41
1:A:317:VAL:CG1	1:A:318:TYR:N	2.84	0.41
2:B:84:THR:HB	2:B:154:LYS:HE2	2.02	0.41
1:A:138:GLU:HG2	1:A:138:GLU:O	2.21	0.41
1:A:274:ILE:HD11	1:A:310:LEU:HD21	2.03	0.41
2:B:149:LEU:HD13	2:B:156:SER:HA	2.02	0.41
2:B:149:LEU:HD21	2:B:159:ILE:HD12	2.02	0.40
1:A:54:ASN:HA	1:A:55:PRO:HD3	1.83	0.40
2:B:270:ILE:HG22	2:B:271:TYR:N	2.35	0.40
1:A:181:TYR:CZ	2:B:138:GLU:HB2	2.57	0.40
2:B:357:MET:CB	2:B:367:GLN:CD	2.90	0.40
1:A:525:LEU:HD23	1:A:531:VAL:HG21	2.03	0.40
1:A:287:LYS:O	1:A:288:ALA:C	2.60	0.40
1:A:12:LEU:HD11	1:A:127:TYR:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	554/556 (100%)	490 (88%)	50 (9%)	14 (2%)	7	18
2	B	411/427 (96%)	353 (86%)	47 (11%)	11 (3%)	6	16
All	All	965/983 (98%)	843 (87%)	97 (10%)	25 (3%)	7	16

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	ILE
1	A	223	LYS
1	A	225	PRO
1	A	334	GLN
1	A	420	PRO
1	A	421	PRO
1	A	458	VAL
1	A	542	ILE
2	B	88	TRP
2	B	140	PRO
2	B	141	GLY
2	B	153	TRP
1	A	104	LYS
1	A	288	ALA
2	B	420	PRO
1	A	52	PRO
1	A	554	ALA
2	B	37	ILE
2	B	277	ARG
2	B	278	GLN
1	A	4	PRO
1	A	413	GLU
2	B	97	PRO
2	B	4	PRO
2	B	270	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	458/496 (92%)	425 (93%)	33 (7%)	18 41
2	B	353/389 (91%)	327 (93%)	26 (7%)	17 39
All	All	811/885 (92%)	752 (93%)	59 (7%)	17 39

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	43	LYS
1	A	48	SER
1	A	72	ARG
1	A	179	VAL
1	A	199	ARG
1	A	210	LEU
1	A	225	PRO
1	A	250	ASP
1	A	284	ARG
1	A	287	LYS
1	A	300	GLU
1	A	303	LEU
1	A	315	HIS
1	A	317	VAL
1	A	330	GLN
1	A	363	ASN
1	A	364	ASP
1	A	385	LYS
1	A	399	GLU
1	A	409	THR
1	A	420	PRO
1	A	422	LEU
1	A	423	VAL
1	A	452	LEU
1	A	459	THR
1	A	475	GLN

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Mol	Chain	Res	Type
1	A	497	THR
1	A	507	GLN
1	A	511	ASP
1	A	516	GLU
1	A	533	LEU
1	A	552	VAL
2	B	6	GLU
2	B	10	VAL
2	B	24	TRP
2	B	42	GLU
2	B	70	LYS
2	B	86	ASP
2	B	94	ILE
2	B	113	ASP
2	B	156	SER
2	B	165	THR
2	B	169	GLU
2	B	176	PRO
2	B	237	ASP
2	B	245	VAL
2	B	248	GLU
2	B	268	SER
2	B	271	TYR
2	B	274	ILE
2	B	290	THR
2	B	293	ILE
2	B	307	ARG
2	B	321	PRO
2	B	394	GLN
2	B	405	TYR
2	B	413	GLU
2	B	414	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	145	GLN
1	A	175	ASN
1	A	198	HIS
1	A	255	ASN
1	A	258	GLN

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Mol	Chain	Res	Type
1	A	306	ASN
1	A	330	GLN
1	A	340	GLN
1	A	361	HIS
1	A	373	GLN
1	A	407	GLN
1	A	474	ASN
1	A	475	GLN
2	B	54	ASN
2	B	57	ASN
2	B	96	HIS
2	B	145	GLN
2	B	147	ASN
2	B	198	HIS
2	B	255	ASN
2	B	278	GLN
2	B	348	ASN
2	B	373	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.